

frac. valid SMILES

1.0  
0.5

frac. unique SMILES

1.0  
0.5

frac. SMILES in train

1  
0

frac. SMILES in PubChem

1.0  
0.5

KLD

0.5  
0.0

Frechet distance

25  
0

frac. SMILES with azo

1  
0

SA score

2.5  
0.0

0.0 0.5 1.0 1.5 2.0  
temperature

